MUONIC MOLECULES OF CHARGE Z≥3: COULOMBIC PROPERTIES AND NUCLEAR TRANSITIONS

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Abstract

In this report we will discuss properties of and models for nuclear transitions in muonic molecules formed via collisions of muonic atoms of hydrogen isotopes with light nuclei like *Li* and *Be*. Their importance for nuclear astrophysics and nuclear physics at super low energies is emphasized.

I. INTRODUCTION

In this report we will mainly consider three particle systems of the type $h\,Li\,\mu$ and $h\,Be\,\mu$, where h= p, d, or t are isotopes of hydrogen, $Li = {}^6Li$ or ${}^7Li$, and $Be = {}^7Be$, ${}^8Be$ or ${}^{10}Be$. There are strong indications that these particles can form molecular three-body resonances which, however, have not yet been observed experimentally. One of these indications is that $d\,He\,\mu$ resonances were seen in collisions of $p\mu$ and $d\mu$ atoms with ${}^3He$ and ${}^4He$ [1]. In the *Li*- or *Be*-case there is, of course, a stronger repulsion (proportional to Z, the charge of the heavy nucleus) which, however, is partly compensated by an attractive force (proportional to Z^2) due to the polarizibility of the $h\mu$ atoms. Theoretical estimations [2–4], in fact, show that $h\,Li\,\mu$ and $h\,Be\,\mu$ resonances do exist. It is however not only the existence, but in particular the formation probability of such systems, which is to be investigated.
Up to now, only mechanisms connected with the transfer of energy to the electronic degrees of freedom in the *Li* or *Be* atom (Auger transitions [5,6] or resonance excitations of atoms in the final state [7]) have been considered in the literature. However, it is to be expected that some other, also resonant, mechanisms exist, leading to the excitation of a (in the Born-Oppenheimer sense) 'slow' degree of freedom. That is, the analog of the Vesman mechanism

[8] for $dt\mu$ formation should play an essential role also in the present case. Indeed, Li atoms are usually not free in a hydrogen medium, but can form molecular hydrides of Li, like LiH, or Li_2 molecules. The whole spectrum of excitations of such molecules is displaced into the region of a few eV. That means, if in the three-particle systems $h\,Li\,\mu$ states exist with a few eV energy, a resonant formation of the Vesman type is possible. This observation explains, why it is so important to perform precise calculations of the spectra of muonic hydrides of Li with the different isotopes of hydrogen and Li. We shall return to this problem later on and discuss the possibility of a realization of the cycling process in a mixture of deuterium and Li.

If the $h\,Li\,\mu$ or $h\,Be\,\mu$ resonances are formed, nuclear transitions can occur in them. Generally, these transitions are expected to be suppressed in comparison with the analogous ones in the $h\,^3He\,\mu$ or $h\,^4He\,\mu$ molecules, simply due to their larger size. However, one can find a few peculiar cases, where the nuclear reactions are of 'long range' in the nuclear scale of distances. There are two reasons for the occurrence of such long-range strong interactions. The first one is related to the presence of a nuclear resonance in the compound systems, close to the threshold energy of some two-body channels and sometimes even in coincidence with it. In other words, long-range nuclear transitions in the molecular system can be expected, when the heavy constituents of a molecule would have a nuclear resonance at zero relative energy. In this case we expect a rather large value for the overlap integral, which characterizes the probability of a transition between the molecular and the nondecreasing nuclear resonance wave functions. As an example of such a situation, we consider the molecule $d\,^7Li\,\mu$. In this case, the resonance state of the $^9Be(5/2^+)$ nucleus occurs near the threshold energy of the two-body channel $d + {}^7Li$. The second reason for long-range nuclear transitions is connected with the occurrence of two closely spaced threshold energies for some two-body channels. It is almost evident that, if transitions between such two channels take place, a small momentum transfer would be transmitted in the transition process, and this implies a long range of the interaction.

As an example of such a situation we consider the threshold energies of the two-body states $d + {}^7Be$ and $p + {}^8Be^*(2^+)$ or $p + {}^{10}Be$ and $t + {}^8Be(g.s.)$. In the first example the difference between the threshold energies of the systems $d + {}^7Be$ and $p + {}^8Be^*(2^+)$ approximately equals $0.04MeV$. In the second example it is equal to $0.004MeV$. Below, we will estimate the probabilities of nuclear transitions in the systems $d\,^7Be\,\mu$ and $p\,^{10}Be\,\mu$.

These systems are of interest also from another points of view. There is a considerable lack of information about the nuclear interactions in the $eV - keV$ energy region. Such energies, however, are attainable in muonic systems. By lack of information, we mean not only that the dynamics of nuclear transitions in this energy interval is not well understood, but also that the validity of the usual properties of the strong interactions is not guaranteed. Properties of strong interactions as charge symmetry, iso-invariance, the character of P- and T-invariance (or its violation) are all established mainly in the MeV region and, up to now, have only been extrapolated to the low-energy region.

A further reason for the interest in such molecules is related to questions of nuclear astrophysics. Here we mean nuclear reactions which took place in the process of primordial nucleosynthesis just after the Big Bang, and those occuring in those stars, where light elements are produced. One of the problems here is the abundance of ^7Li in the Universe. In order to discuss this problem reliably, we first establish that the abundance of ^7Li seen in

the Universe is indeed due to primordial nucleosynthesis. Evidence for this conjecture was found some years ago from the observation of the abundance of ^7Li in old stars [9].
In Figure 1 the abundance of ^7Li is shown as a function of the abundance of Fe. It can be compared with the abundance of Mg (see Figure 2), an element which was definitely not created in primordial nucleosynthesis, but in the stars.
This comparison indeed indicates that the abundance of ^7Li nuclei, in contrast to the case of Mg, is constant and therefore cannot be attributed to the processes occuring in the stars. The modern theory [10] of the creation of light elements during the primordial nucleosynthesis, predicts the following distributions as functions of the nucleon-to-photon ratio η.
In this theory one has to use the cross sections for the nuclear reactions in the keV range of energies. These energies are not accessible in laboratory experiments, when we want to study for instance reactions involving ^7Li nuclei, such as

$$p + {}^7Li \longrightarrow 2\,\alpha$$
$$\text{and } t + \alpha \longrightarrow {}^7Li + \gamma\ .$$

We can try to get access to these data via the the observation of such transitions in the muonic systems $p\,{}^7Li\,\mu$ and $t\,{}^4He\,\mu$

$$p\ {}^7Li\,\mu \longrightarrow \left\{ \begin{array}{l} {}^8Be\,\mu + \gamma \\ {}^8Be + \mu \end{array} \right.$$

and

$$t\ {}^4He\,\mu \longrightarrow \left\{ \begin{array}{l} {}^7Li\,\mu + \gamma \\ {}^7Li + \mu \end{array} \right. ,$$

where the relative energy of the heavy particles in the molecule is arround a few eV only.
Usually, astrophysicists extrapolate the astrophysical S-factor[1], defined as

$$\sigma = \frac{e^{-2\pi\eta(E)}}{E} S(E)\ , \tag{1}$$

into the region of low energies. How dangerous such a process is, can be seen from the example of the extrapolation procedure for the S-factor of the reaction

$$d + d \longrightarrow {}^4He + \gamma\ . \tag{2}$$

In Figure 4 we show the extrapolated S-factor and the S-factor, fitted to the new data at low energies [11]. It is seen that the difference in the 'old' and 'new' S(0)-values is two orders of magnitude.
Another reaction that we discuss in the context of muonic systems is the radiative capture of protons by the ^7Be nucleus

$$p + {}^7Be \longrightarrow {}^8B + \gamma\ . \tag{3}$$

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[1]The S-factor is assumed to be a slow function of the energy, if no resonances in the region concerned are present.

It is well known [12] that this transition is the last step in the pp-chain in the sun and is the bottleneck, which is crucial for the determination of the flux of high energy neutrinos from the sun [13]. In laboratory measurements of the cross section of this process only the region of energies down to $100keV$ is accessible. An extrapolation to the energies at the centre of the sun ($1.5keV$) has to be made. Here again one of the possibilities to obtain the value of the S-factor in the few eV energy region is to search for this transition in the muonic molecule $p\,^7Be\,\mu$. In this case we do not have a threshold resonance in the $p + {}^7Be$ system, but a very peculiar final state. The wave function of the ground state of the ^8B nucleus has a very long tail due to the (on a nuclear scale) extremely small separation energy of the proton in ^8B, which equals to $0.14MeV$. Due to this long tail, we again have a process, which occurs at large distances and can be favourable for its observation in the muonic system $p\,^7Be\,\mu$.

II. THEORETICAL DESCRIPTION OF CHARGE NONSYMMETRIC MUONIC MOLECULES

In this chapter we describe the treatment of the three-body Coulomb problem $hZ\mu$. Since we have two heavy particles and one light particle, it seems that the Born-Oppenheimer approach will be reasonable to describe this system. Indeed, some estimations [2] of the properties of the $h\,He\,\mu$ systems performed by this method (in the one-channel approximation) provided a qualitatively correct description of some properties. Of course, the quantitative description requires improvements since, within this approximation, it is impossible to reproduce even the spectra of the usual muonic molecules of hydrogen. Moreover, since we are interested in the probabilities of some partial transitions, say the probability of formation, it will be more reliable to use a method taking angular momentum conservation into account. Another problem within the framework of the Born-Oppenheimer approach is that it is very difficult to treat the contribution from the continuum spectra of the two-center problem correctly. Thus, to avoid these difficulties we will use another adiabatic formulation, namely the hyperspherical adiabatic approach [14,15]. This method is based on an expansion of the three-body wave function into the so-called surface functions [16].
Let us start the description of our formalism regarding Figure 5, where the Jacobi coordinates are shown.
In these variables the Hamilton operator of the three-body Coulomb system takes the form

$$H = -\frac{1}{2m}\Delta_{\vec{r}} - \frac{1}{2M}\Delta_{\vec{R}} - \frac{Ze^2}{r} - \frac{e^2}{|\vec{R} - \beta\vec{r}|} + \frac{e^2}{|\vec{R} + \gamma\vec{r}|}\,, \tag{4}$$

where

$$m^{-1} = m_\mu^{-1} + m_Z^{-1}, \quad M^{-1} = m_h^{-1} + (m_\mu + m_Z)^{-1}, \quad \beta = \frac{m_Z}{m_\mu + m_Z}, \quad \gamma = 1 - \beta \tag{5}$$

and m_μ, m_h and m_Z denote the masses of the muon, the hydrogen isotop and the heavier nucleus (with charge Z), respectively. Introducing dimensionless variables according to

$$\vec{x} = \frac{\vec{r}}{a}, \quad \vec{y} = \frac{\vec{R}}{\alpha a}\,, \tag{6}$$

with $\alpha = \sqrt{\frac{m}{M}}$ and a being the Bohr radius of the $(Z\mu)$ subsystem, $a = (Zme^2)^{-1}$, the Hamiltonian reads

$$H = \frac{1}{2ma^2}\left\{ -\Delta_{\vec{x}} - \Delta_{\vec{y}} - \frac{2}{x} - \frac{2}{Z|\alpha\vec{y} - \beta\vec{x}|} + \frac{2}{Z|\alpha\vec{y} + \gamma\vec{x}|} \right\} . \tag{7}$$

This suggests to take $(2ma^2)^{-1}$ as our energy unit. Let us define the hyperradius ρ and the hyperangle ω via

$$x = \rho\cos\omega, \quad y = \rho\sin\omega \ , \tag{8}$$

with $0 \le \rho < \infty$ and $0 \le \omega \le \pi/2$. The Hamiltonian (7) then takes the well-known form

$$H = -\rho^{-5/2}\frac{\partial^2}{\partial\rho^2}\rho^{5/2} + \frac{\Lambda^2(\Omega)}{\rho^2} + \frac{\mathcal{V}(\Omega)}{\rho} \ , \tag{9}$$

where the grand angular momentum operator $\Lambda(\Omega)$ is given by

$$\Lambda^2(\Omega) = -\frac{1}{\cos\omega\sin\omega}\frac{\partial^2}{\partial\omega^2}\cos\omega\sin\omega + \frac{\vec{l}^{\,2}_{\hat{x}}}{\cos^2\omega} + \frac{\vec{l}^{\,2}_{\hat{y}}}{\sin^2\omega} - \frac{1}{4} \ . \tag{10}$$

$\vec{l}_{\hat{x}}$ and $\vec{l}_{\hat{y}}$ are the orbital angular momentum operators corresponding to the variables $\hat{x} = \vec{x}/x$ and $\hat{y} = \vec{y}/y$, respectively. For the potential we have

$$\mathcal{V}(\Omega) = -2\left\{ \frac{1}{\cos\omega} + \frac{1}{Z|\alpha\hat{y}\sin\omega - \beta\hat{x}\cos\omega|} - \frac{1}{Z|\alpha\hat{y}\sin\omega + \gamma\hat{x}\cos\omega|} \right\} . \tag{11}$$

The five angles symbolized by $\Omega = (\omega, \hat{x}, \hat{y})$ together with the hyperradius ρ provide a complete set of variables to describe the positions of all three particles. The Schrödinger equation therefore is

$$\left\{ -\rho^{-5/2}\frac{\partial^2}{\partial\rho^2}\rho^{5/2} + \frac{\Lambda^2(\Omega)}{\rho^2} + \frac{\mathcal{V}(\Omega)}{\rho} \right\} \Psi(\rho,\Omega) = E\ \Psi(\rho,\Omega) \ . \tag{12}$$

Let us now introduce the surface functions mentioned above. We want to use these functions as a basis for the solutions $\Psi(\rho,\Omega)$ of (12). For this purpose we consider the operator containing only the angular part of the Hamiltonian,

$$\left\{ \frac{\Lambda^2(\Omega)}{\rho^2} + \frac{\mathcal{V}(\Omega)}{\rho} \right\} B_n(\rho,\Omega) = U_n(\rho)\ B_n(\rho,\Omega) \ . \tag{13}$$

Its eigenfunctions $B_n(\rho,\Omega)$ are the so-called *surface functions*, its eigenvalues $U_n(\rho)$ are called *eigenpotentials*. In equation (13) the hyperradius ρ enters only as a parameter. Since the surface functions form a complete set on the sphere of constant values of the hyperradius, the three-body wave function can be expanded according to

$$\Psi(\rho,\Omega) = \rho^{-5/2}\sum_n f_n(\rho)B_n(\rho,\Omega) \ . \tag{14}$$

The adiabatic approximation consists in the truncation of this sum into a finite number of terms. In contrast to the Born-Oppenheimer approach, not the distance between the two heavy particles, but the hyperradius (a measure of the average size of the whole system) is the 'slow' variable. Both variables coincide if the mass of the light particle (here m_μ) tends to zero. The two major advantages of our approach, in comparison with the Born-Oppenheimer one, are that here the total angular momentum is a good quantum number and that the eigenpotentials $U_n(\rho)$ tend to the exact two-body binding energies in the limit of $\rho \longrightarrow \infty$. Both properties can be derived from equation (13).
Instead of solving the coupled system of differential equations, which is obtained by inserting (14) into the Schrödinger equation (12), we here only treat the so-called *extreme adiabatic approximation*, which is given by the neglect of the derivatives of the surface functions with respect to the hyperradius. The remaining radial equation then is

$$f_n''(\rho) = [U_n(\rho) - E] f_n(\rho) \; , \tag{15}$$

looking exactly as a radial two-body Schrödinger equation, where $U_n(\rho)$ acts as an effective potential. Hence the name 'eigenpotential'.
The main task now consists in the determination of these eigenpotentials. As it can be seen from equation (13), for small values of the hyperradius, Λ^2/ρ^2 dominates over the Coulomb potential $\mathcal{V}/\rho$. Therefore, the surface functions in this region should be proportional to the eigenfunctions of Λ^2, which are the well-known [17] hyperspherical harmonics $Y_{[\mathcal{L}]}(\Omega)$

$$Y_{[\mathcal{L}]}(\Omega) = N_{[\mathcal{L}]} \; \cos^{l_x}\omega \; \sin^{l_y}\omega \; P_k^{(l_y+\frac{1}{2}, l_x+\frac{1}{2})}(\cos 2\omega) \; \mathcal{Y}_{l_x l_y}^{LM}(\hat{x}, \hat{y}) \; . \tag{16}$$

These functions are characterized by the set of quantum numbers $[\mathcal{L}] = \{k, l_x, l_y, L, M\}$. They contain the Jacobi polynomial

$$P_k^{(\alpha,\beta)}(x) = \frac{(x-1)^{-\alpha}(x+1)^{-\beta}}{2^k k!} \frac{d^k}{dx^k} \left[(x-1)^{k+\alpha}(x+1)^{k+\beta} \right] \tag{17}$$

and the bispherical harmonics (eigenfunctions of the squared total angular momentum operator $\vec{L}^2$)

$$\mathcal{Y}_{l_x l_y}^{LM}(\hat{x}, \hat{y}) = \sum_{m_x m_y} \langle \, l_x m_x l_y m_y \, | \, LM \, \rangle \; Y_{l_x m_x}(\hat{x}) \; Y_{l_y m_y}(\hat{y}) \tag{18}$$

with the Clebsch-Gordan coefficients $\langle \, l_x m_x l_y m_y \, | \, LM \, \rangle$. The normalization constant $N_{[\mathcal{L}]}$ is given by

$$N_{[\mathcal{L}]} = \sqrt{\frac{2k! \; (l_x + l_y + 2k + 2) \; \Gamma(l_x + l_y + k + 2)}{\Gamma(l_x + k + \frac{3}{2}) \; \Gamma(l_y + k + \frac{3}{2})}} \; . \tag{19}$$

Large values of the hyperradius and negative energies (the only energies we are interested in) correspond to the physical situation where the muon is bound by one of the positive charges. Hence, the surface functions in this region look like channel functions [18]

$$\Phi_{[m_i]}(\rho, \Omega) = \rho^{3/2} \; \mathcal{R}_{n l_x}(\rho \cos\omega) \; \sin^{l_y}\omega \; \mathcal{Y}_{l_x l_y}^{LM}(\hat{x}, \hat{y}) \; . \tag{20}$$

Here, $\mathcal{R}_{nl_x}(x)$ denotes a hydrogen-like wave function and $[m]$ the set of quantum numbers $\{n, l_x, l_y, L, M\}$. The index 'i' specifies by which of the two nuclei the muon is bound.
To represent the surface functions in the whole space of ρ we use the following ansatz

$$B_n(\rho,\Omega) = \sum_{i=1}^{2} \sum_{[m_i]} a_{n[m_i]}(\rho)\ \Phi_{[m_i]}(\rho,\Omega)\ +\ \sum_{[\mathcal{L}]} b_{n[\mathcal{L}]}(\rho)\ Y_{[\mathcal{L}]}(\Omega)\ , \tag{21}$$

which (inserted in equation (13)) yields a generalized eigenvalue problem for the determination of the coefficients $a_{n[m_i]}(\rho)$ and $b_{n[\mathcal{L}]}(\rho)$ and the eigenpotentials $U_n(\rho)$.
Within this framework we treated the systems $dt\mu$, $h\,^6Li\,\mu$, $h\,^7Li\,\mu$ and $h\,^7Be\,\mu$ in the states with the total angular momentum $L = 0$. In all calculations we use 120 hyperspherical functions (16). In the case of $(dt\mu)$ we take 6 channel functions (20) and for the systems of higher charge we take 10 channel functions into account. The latter is useful due to the higher polarizibility of the $(h\mu)$ atom by the nucleus of higher charge. Tables I to IV show the binding energies of the various muonic molecules using the extreme adiabatic approximation (15) in comparison with the results of References [5,19].

III. ESTIMATIONS OF NUCLEAR TRANSITION PROBABILITIES IN MUONIC MOLECULES OF BE ISOTOPES

We start by considering simpler systems with respect to their nuclear structure, e.g. the system $d\,^7Be\,\mu$, to demonstrate the approximations we make and to discuss their reliability [20]. First, consider the structure of the spectrum of the ^8Be nucleus shown in Figure 6.
As one can immediately see that is the case of two thresholds close to each other, which correspond to the states $d +\ ^7Be$ and $p +\ ^8Be(2^+)$. The difference between these threshold energies is equal to $0.044MeV$, a very small value on the nuclear scale. In such a way, if the nuclear transition $d +\ ^7Be \longrightarrow p +\ ^8Be(2^+)$ takes place, only a small momentum transfer is possible and large distances between d and ^7Be are involved.
Now, let us formulate the description of such a transition in the muonic system

$$d\,^7Be\,\mu \longrightarrow p\,^8Be(2^+)\,\mu\ . \tag{22}$$

We will treat both states (initial and final) as four-body systems $n + p +\ ^7Be + \mu$. The internal structure of the ^7Be nucleus is not important in the range of energy and momentum transfer involved. For that reason we will treat the excited state of the $^8Be(2^+)$ nucleus in a simple two-body $n +\ ^7Be$ model. Let us introduce the two sets of Jacobi coordinates, shown in Figure 7, which are appropriate for the description of the initial and final states.
The total Hamiltonian can be written in the form

$$H = H_0 + V^C + V^S\ , \tag{23}$$

where the sum of the kinetic energies H_0 is given by

$$H_0 = h_0(\vec{r}) + h_0(\vec{\rho}) + h_0(\vec{R})\ , \tag{24}$$

and the potentials of the Coulomb, V^C, and strong, V^S, interactions are

$$V^C = V^C_{^7Be\mu} + V^C_{p\mu} + V^C_{p\,^7Be} \qquad \text{and} \qquad V^S = V^S_{np} + V^S_{n\,^7Be} + V^S_{p\,^7Be} \ , \tag{25}$$

respectively. To continue, it is useful to introduce the auxiliary channel Hamiltonians $H_{1,2}$, defined via

$$\begin{aligned} H_1 = {} & h_0(\vec{r}_1) + h_0(\vec{\rho}_1) + h_0(\vec{R}_1) + V^S_{np}(\vec{r}_1) \\ & + V^C_{^7Be\mu} + V^C_{d\mu} + V^C_{d\,^7Be} \end{aligned} \tag{26}$$

and

$$\begin{aligned} H_2 = {} & h_0(\vec{r}_2) + h_0(\vec{\rho}_2) + h_0(\vec{R}_2) + V^S_{n\,^7Be}(\vec{r}_2) \\ & + V^C_{^8Be\mu} + V^C_{p\mu} + V^C_{p\,^8Be} \ , \end{aligned} \tag{27}$$

and the corresponding Schrödinger equations for the channel eigenfunction[2],

$$H_i\psi_i = \varepsilon_i\psi_i \ , \qquad i = 1, 2 \ . \tag{28}$$

As one can see from the equations (26) and (27) the channel Hamiltonians do not contain the strong interaction between the clusters d and ^7Be in the initial state and between p and ^8Be in the final one. Therefore they describe the three-body Coulomb systems $d\,^7Be\,\mu$ and $p\,^8Be\,\mu$ and the internal motions in the deuteron and ^8Be nucleus, and therefore are still four-body Hamiltonians.
To solve the Schrödinger equation

$$H\Psi = E\Psi \tag{29}$$

with the full Hamiltonian (23) we use the ansatz

$$\Psi = c_1\psi_1 + c_2\psi_2 \ . \tag{30}$$

This ansatz reminds us of the well-known LCAO (Linear Combination of Atomic Orbitals) approximation, where the role of the 'atomic orbitals' is played by the nuclear states of d and $^8Be(2^+)$. The approximation (30) therefore implies that the internal motion in the deuteron does not disturb the internal motion in the ^8Be nucleus much and vice versa. Let us discuss the reliability of that ansatz for the solution of equation (29). We should first note that in the usual molecular ion of the hydrogen H_2^+, where the LCAO approximation is qualitatively a good one, the size of the atomic orbital has the same order of magnitude as the size of the H_2^+ ion itself, namely $r_0 \sim 10^{-8}cm$. In the case of the muonic system the 'orbitals' (d and $^8Be(2^+)$) are of a nuclear size ($\sim 10^{-13}cm$) and the $d\,^7Be\,\mu$ molecule has a size of $\sim 10^{-9}cm$ [15]. So the orbitals in our case are four orders of magnitude smaller than the molecule and we should expect much more reliable results from approximation (30) than in the case of the H_2^+ ion. To continue the analogy with the H_2^+ ion we consider the picture, in which the

[2]For reasons of simplicity we will neglect for the moment the contributions from the non-point-like charge distributions in the d and ^8Be nuclei.

neutron can be bound in some potential well by the proton (position a) or almost with the same binding energy by the ^7Be nucleus (position b), as is shown in Figure 8.
It is well-known in quantum mechanics that in such systems, where the possibility exists that a particle can be present in either of the two potential wells, splitting of levels should occur. This does indeed happen to a significant extent in this case as we shall now proceed to demonstrate. From the structure of the channel Hamiltonians $H_{1,2}$ we immediately find for the eigenfunctions $\psi_{1,2}$ that

$$\psi_1 = \Phi_d(\vec{r}_1) \;\; \Phi_1^{mol}(\vec{\rho}_1, \vec{R}_1) \tag{31}$$

and

$$\psi_2 = \Phi_{^8Be}(\vec{r}_2) \;\; \Phi_2^{mol}(\vec{\rho}_2, \vec{R}_2) \; . \tag{32}$$

Here Φ_d and $\Phi_{^8Be}$ are wave functions, which describe the internal motion in the d and $^8Be(2^+)$ nuclei, while the molecular functions for $d\,^7Be\,\mu$ and $p\,^8Be\,\mu$ are given by Φ_1^{mol} and Φ_2^{mol}, respectively.
Now, after diagonalization of the total four-body Hamiltonian H with the basis functions (31) and (32), we easily find the coefficients c_1 and c_2 in equation (30) and the transition matrix element M,

$$M \sim \langle\, \Psi \,|\, \psi_2 \,\rangle \; . \tag{33}$$

For the reaction rate P we then have

$$P = \kappa |\langle\, \Psi \,|\, \psi_2 \,\rangle|^2 \; , \tag{34}$$

where κ is the muonic molecule frequency. It is easy to see that we obtain two solutions of equation (29), $\Psi^{\pm}$, corresponding to the split levels $E^{\pm}$,

$$\Psi^{\pm} = N^{\pm}(\lambda^{\pm}\psi_1 + \psi_2) \; , \tag{35}$$

where $N^{\pm}$ is the normalization constant and

$$\lambda^{\pm} = \frac{E^{\pm} I - H_{12}}{H_{11} - E^{\pm}} \; , \tag{36}$$

with the matrix elements

$$I = \langle\, \psi_1 \,|\, \psi_2 \,\rangle \qquad \text{and} \qquad H_{ij} = \langle\, \psi_i \,|\, H \,|\, \psi_j \,\rangle \; , \tag{37}$$

which are indeed multidimensional integrals. For the transition rate (34) we obtain

$$P^{\pm} = \kappa \frac{|1 + I^* \lambda^{\pm}|^2}{1 + 2Re(I^* \lambda^{\pm}) + |\lambda^{\pm}|^2} \; . \tag{38}$$

From the structure of the channel functions (31) and (32) it is easy to see that for the overlap integral I we have the relation

$$I = \langle\, \psi_1 \,|\, \psi_2 \,\rangle \sim \int d\vec{\rho} \;\; |\Phi^{mol}(\vec{\rho}, R = 0)|^2 \;\; = \;\; S_3 \; , \tag{39}$$

where the value of S_3 can be interpreted as a probability for the heavy particles in muonic molecules to be at small distances (zero distance in this case). It is easy to see that the matrix elements of the total four-body Hamiltonian (23) also can be expressed through the overlap integral (39). For example for H_{11} we have

$$H_{11} \approx \varepsilon_1 + S_3(V^{11}_{n\,Be} + V^{11}_{p\,Be}) \; , \tag{40}$$

where the V^{11}_{NBe} are the matrix elements of the strong NBe potentials over the wave function of the deuteron Φ_d.
Since the nuclear V_{NBe} potentials have been determined by experimentall data [22], the most uncertain value, defining the rate (38) of the nuclear transition, is S_3, the probability for the heavy particles to be close to each other. To make a rough estimation we will proceed in the following way. On a qualitative level the three-body muonic states like $p\,Be\,\mu$ can be considered as two-body $(p + Be)$ systems, moving in an effective potential produced by the muon. In that potential we can calculate the probability for the heavy particles to be at small distances. Let us call this value S_2. Then we can suppose that

$$S_3 \approx S_2 = |\Phi(R = 0)|^2 \; , \tag{41}$$

The value of the wave function at small distances can be estimated [23] as

$$|\Phi(R = 0)|^2 \leq (m\ \Delta E)^{3/2} \; . \tag{42}$$

Here m is the reduced mass of the two particles and ΔE the separation between the s and p levels in the effective potential, which produces the wave function $\Phi(R)$. Using this estimation for the rate of the nuclear transition P^-, the only one available in the process $d\,^7Be\,\mu \longrightarrow p\,^8Be\,\mu$, one obtains [20]

$$P^- = 4.6 * 10^{11} sec^{-1}. \tag{43}$$

The inequality (42) probably overestimates the real value, since the repulsion in the effective potential is not fully specified in Reference [23].

Now let us come to the description of the nuclear transition in the molecule $p\,^{10}Be\,\mu$ [24]

$$p\,^{10}Be\,\mu \longrightarrow t\,^8Be\,\mu + Q \; , \qquad\qquad Q \approx 4keV \; . \tag{44}$$

The incredibly small energy release in this transition is related to the peculiar properties of the ^{10}Be nucleus. Indeed, as one can see from Figure 9, a double coincidence takes place here: the coincidence of the position of the excited state $8.4774MeV$ with the threshold energy in the channel $^8Be + 2n$, and a coincidence of the absolute value of the energy of this excited state with the binding energy of the triton $(8.48MeV)$.
An additional peculiarity of that transition, in comparison with the previous one, can be seen from the spectrum of the ^{11}B nucleus. It turns out that this nucleus has excited states with energies which coincide with the threshold energy in the channel $p + {}^{10}Be$. Keeping this in mind, two essentially different mechanisms of the transition can be formulated, as shown in Figures 10 and 11.

However, since the spins of the corresponding excited states of the nucleus ^{11}B are rather high ($9/2^+$,$5/2^-$), we will neglect contributions from that mechanism. In other words, our transition amplitude does not contain the resonant term from Figure 11, due to a sufficiently small angular momentum in the initial state. So, we can proceed in complete analogy with the previous case. The only complications which arise, are due to the more complex wave function of the nuclear state. To describe the process in the frame of the 'LCAO' ansatz, we have used a four particle ($2\alpha + 2n$) model for the description of the ground state of the ^{10}Be nucleus, and a 2α model for $^{8}Be(g.s.)$.
All we need now are $N\alpha$ and NN potentials, wave functions of the nuclei $^{10}Be(g.s.)$, $^{8}Be(g.s.)$ and the triton and molecular wave functions at small distances. The nuclear wave functions were written in a simple form, reproducing only the periphery of the nuclei [25,26]. For the $N\alpha$ potentials three different but phaseshift equivalent potentials [27–29] were applied. The results are sensitive to the differences in their shape. The molecular wave function was constructed by means of the potential

$$V(R) = 4.5\,H\,[\frac{2}{\pi}\arctan(aR) - 1]\,e^{-bR} - 8\,H\ , \tag{45}$$

with parameters fitted to the eigenpotential calculated by means of the method of surface functions [15]. Here, $H = me^4/\hbar^2 = 5626.5eV$ is the Hartree energy unit for the muon. The potential (45), of course, produces a more reliable wave function of the molecule at small distances as compared to the estimation of equation (42). As NN potentials the Malfliet-Tjon potentials [30] have been used. The results for the reaction rates are shown in Table V. The fact that the lowest reaction rate occurs with the $N\alpha$ potential given in Reference [29], most likely is a reflection of the repulsive character of that potential.

IV. NEW CYCLING PROCESSES AND OTHER SPECULATIONS

Considering the properties of molecular systems with isotopes of Li nuclei, we can hope that, in principle, new cycles analogous to the one occuring in the dt mixture, can take place. To see this analogy more clearly, let us remind ourselves of the picture of the cycle with the $dt\mu$ molecule, as shown in Figure 12.
Roughly speaking, the two following parameters of that cycle are specific only for this system: 1) the probability of the resonant formation of the $dt\mu$ excited state[3], 2) the probability of a nuclear transition in the $dt\mu$ molecule which also has a resonance behavior. As it was pointed out in the introduction, the possibility of resonance formation of $d\,Li\,\mu$ systems cannot be excluded in collisions of the type $d\mu + LiD$. If excited states in $d\,Li\,\mu$ systems within the energy range $E \leq 2.5eV$ exist, the Vesman mechanism can be invoked. ($E \approx 2.5eV$ is the dissociation energy of the molecule LiD from the $A'\Sigma^+$ state [32]).
Considering the nuclear resonances we see for both isotopes of Li a situation, which might be even more favourable for nuclear transitions than in the $dt\mu$ case. Indeed, let us look on the spectra of the nuclei ^{8}Be and ^{9}Be, schematically shown in Figures 13 and 14, respectively.

[3]Resonance molecular formation, as it is well-known [31], also takes place in $d\mu + D_2$ collisions.

We see that in both cases there are threshold resonant states in the compound nuclei ^8Be and ^9Be and the positions of these resonances are closer to the corresponding thresholds than the position of the $^5He(3/2^+)$ resonance to the $d+t$ threshold. In the last case the 'center' (on the energy scale) of the resonance state $^5He(3/2^+)$ is $50keV$ higher than the threshold energy. A nuclear transition, therefore, only takes place through the tail of the resonance curve. Keeping in mind the above pecularities of the molecular and nuclear structures of the systems $d\mu + {}^{6,7}Li$, we can imagine the cycle in the $d+Li$ mixture, shown in Figure 15. The third parameter crucial for the occurence of the cycling process is the sticking coefficient for the muon in the final state. Unfortunately, none of these three parameters have till now reliably estimated.

Other interesting phenomena can be observed in the above systems. We are talking about the so-called Zeldovich phenomenon or rearrangement of the spectra of Coulomb systems by a short range interaction. As it was shown by Zeldovich [33], in systems with long and short range interactions a rearrangement of the spectrum of the purely long range potential takes place, if the short range interaction has a resonance or bound state near zero energy. In this case the strong interaction cannot be treated perturbatively despite its short range character. Both muonic systems $d\,^6Li\,\mu$ and $d\,^7Li\,\mu$ are indeed good candidates for the manifestation of the Zeldovich phenomenon, since the short range nuclear interactions must generate a resonance behavior at zero relative energy of d and Li. It is necessary to emphasize that the rearrangement of the spectra takes place due to the large size of the hadronic subsystem at the conditions we have described above.
Considering the nonperturbative situation concerning the influence of the strong interaction, we can look for the possibility of nuclear transitions in the corresponding electronic molecules. As an example let us consider a molecule of ordinary light water, $H_2\,^{16}O$. An interesting property of that molecule is the coincidence of its energy with the energy of the excited state of the nucleus ^{18}Ne. Let us look at the spectrum of this nucleus, schematically shown in Figure 16.
As one can see, the nucleus ^{18}Ne indeed has a state with an energy incredibly close (within the accuracy of all measurable figures [35]) to the treshold energy for the three-body channel $^{16}O+2p$. Since the binding energy of water is only a few eV, we claim that the water molecule in the rotational state 1^- and the nucleus ^{18}Ne in the excited state (1^-) of $4.522MeV$ are degenerate states of the same Hamiltonian, describing 18 nucleons and 10 electrons. This implies that the wave function of molecular water is not a pure state, but always contains an admixture of the nuclear state. Since this excited state of the ^{18}Ne nucleus can decay to other channels, for example, in the channel $^{17}F+p$, molecular water should slowly disappear through the resonance state of the nucleus ^{18}Ne. In other words, the smouldering (slow burning) of water should take place with an intensity defined by the overlap of the molecular wave function and the nondecreasing wave function of the resonance nuclear state. Exactly the same is valid for the molecules of hydrides of Li due to the coincidence of the nuclear resonance and threshold energies.

V. CONCLUSIONS AND OUTLOOK

In this paper we reviewed work performed by our group during the last few years, devoted to charge nonsymmetric muonic molecules. For their treatment we have to consider both Coulombic and nuclear few-body problems. We have given special attention to examples where the interplay between the Coulomb forces and the nuclear forces is of atmost importance. We have performed calculations for some of these examples which have been reviewed here and others will be published elsewhere.

For the treatment of the purely Coulombic systems, we employed the method of hyperspherical surface functions. We have calculated eigenpotentials and eigenfunctions for all isotopes of hydrogen and Li and some isotopes of Be. Using the extreme adiabatic approximation, our calculations yield no loosely bound states ($\sim$ 1 or $2eV$) having total angular momentum $L = 0$. The nuclear transitions were calculated in a scheme motivated by the LCAO method, but improved by taking into account all degrees of freedom of light and heavy particles. To reduce the numerical effort to manageable proportions we introduced effective potentials between the nuclear clusters. Obviously, there is a degree of nonuniqueness in this procedure. However the main features entering into our calculations, like the positions of the thresholds, are not effected by this approximation.

We have considered nuclear transitions in the molecules $d\,^7Be\,\mu$ and $p\,^{10}Be\,\mu$, where the energy releases as well as the momentum transfers are extremely small on the nuclear scale. For these reasons the nuclear interactions are expected to have a long range character, which is important in muonic systems.

We now briefly discuss the reliability of the nuclear reaction rates performed in these two cases. The crucial ingredient in these calculations is the value of the molecular wave function at the origin. In the first instance we calculated this quantity by using a rather crude approximation, where the Coulomb interactions were only taken into account in an indirect way suggested by Ref. [23]. In the second example the Coulomb repulsion at short distances was taken into account rather reliably, since the eigenpotentials obtained via the hyperspherical surface function method have the correct behavior near the origin.

To proceed further we have to keep in mind the difficulties associated with the Coulombic three-body problem in which we are interested. In the first place we should emphasize that the systems of the type $hZ\mu$ with $Z \geq 3$ are highly excited resonances and up to now no complete solution of neither the Schrödinger equation nor the Faddeev equations has been presented anywhere. The difficulties of the solution of the Schrödinger equation are related mainly to the very complicated boundary conditions in the configuration space. Faddeev equations for Coulomb forces are not of Fredholm type in this range of energies and should therefore be modified to obtain unique solutions. Additional difficulties arise from the fact that the calculations of the eigenvalues must be performed to a very high accuracy. As indicated above, the dissociation energies of the molecule LiD lie around $2.5eV$. That means that the accuracy of the calculated binding energies of the systems $d\,Li\,\mu$ should be of the order of $1eV$ or even better.

It seems that at the present time only two approaches are sufficiently promising for the treatment of such systems. The first one is the hyperspherical surface function expansion, briefly presented here. From physical reasons we consider resonance states in the extreme adiabatic approximation as real bound states having no width. Indeed, the inclusion of

the coupling between the channels corresponds to taking very high excitation energies into account. The width appears only, when nonadiabaticity is taken into account and a coupled system of equations is employed.
The second promising method, which is very often used in molecular physics [36], also is based on the treatment of the resonance state as a bound state. But the realization of that idea is more motivated by mathematical arguments. To get a square integrable solution in this approach, we use coordinate rotation in the complex plane. It can be shown [36] that the rotated Hamiltonian has the same eigenvalues as the physical one.
Concerning the study of the nuclear interaction in the $eV - keV$ energy region, one can say that it is the only region of energies in the field of nuclear physics, where there are practically no data available. We emphasize that the research proposed here can shed light on the properties and behavior of nuclear systems and interactions in the very far periphery at distances, exceeding the usual range of the nuclear interaction by several orders of magnitude, if one considers muonic systems.

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TABLES

TABLE I. Binding energies of $(dt\mu)$ with $L = 0$

state	ground state	excited state
present	-295.54	-35.80
[19]	-319.14	-34.83

TABLE II. Binding energies of $(h\,^6Li\,\mu)$ with $L = 0$

system	$p\,^6Li\,\mu$	$d\,^6Li\,\mu$	$t\,^6Li\,\mu$
present	-24.3	-23.8	-35.3
[5]	-17.6	-18.5	-19.8

TABLE III. Binding energies of $(h\,^7Li\,\mu)$ with $L = 0$

system	$p\,^7Li\,\mu$	$d\,^7Li\,\mu$	$t\,^7Li\,\mu$
present	-20.8	-25.9	-37.5
[5]	-21.0	-22.0	-23.3

TABLE IV. Binding energies of $(h\,^7Be\,\mu)$ with $L = 0$

system	$p\,^7Be\,\mu$	$d\,^7Be\,\mu$
present	-11.7	-29.3

TABLE V. Reaction rates for the transition $p\,^{10}Be\,\mu \longrightarrow t\,^8Be\,\mu$ calculated with the three different αN potentials [27–29].

Potential	[27]	[28]	[29]
$P^-[sec^{-1}]$	1688	1129	238

Figure Captions.

FIG.1. The correlation between the abundance of Li and Fe in old stars (normalized to the abundance in the sun).

FIG.2. The correlation between the abundance of Mg and Fe in old stars (normalized to the abundance in the sun).

FIG.3. Y_P denotes the predicted primordial abundance of ^4He relative to H as a function of η for three different numbers of neutrino species N_ν. The other curves show the relative abundances of D, ^3He, and ^7Li as a function of η.

FIG.4. New experimentall data (at energies less than $100keV$) and old data (above $100keV$) for the S-factor. The full calculation (solid line) is shown together with a calculation using only the ($L = 2$,$S = 2$) configuration (short-dashed line).

FIG.5. Jacobi coordinates for the system $hZ\mu$.

FIG.6. The spectrum of the ^8Be nucleus (schematically) [21].

FIG.7. Two different sets of Jacobi coordinates appropriate to describe the initial and the final states of the four-body system.

FIG.8. a) The neutron is bound by the proton b) it is bound by the ^7Be nucleus.

FIG.9. The spectrum of the ^{10}Be nucleus (schematically) [21].

FIG.10. Transition through the transfer of two neutrons.

FIG.11. Transition through the resonance state of the $^{11}B^*$ nucleus.

FIG.12. The basic reactions of the muon catalyzed dt fusion cycle.

FIG.13. The excited state of ^8Be and the position of the threshold for the decay into $d+\ ^6Li$ [21].

FIG.14. The excited state of ^9Be and the position of the threshold for the decay into $d+\ ^7Li$ [21].

FIG.15. The basic reactions of the muon catalyzed $d\ ^{6,7}Li$ fusion cycle.

FIG.16. The excited state of ^{18}Ne and the position of the threshold for the decay into $^{16}O+2p$ [34].

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